Connecting via Winsock to STN

Welcome to STN International! Enter x:x
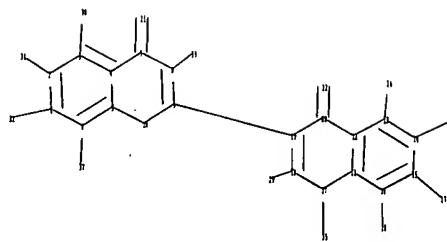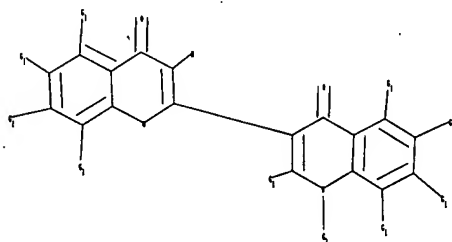
* * * * * * * * * * STN Columbus * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007

=> file reg

=>
Uploading C:\Program Files\Stnexp\Queries\10519208.str

chain nodes :
21 22 24 25 27 28 29 30 31 32 35 37 39
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
1-32 2-31 3-30 6-37 7-21 8-39 9-19 13-24 14-25 15-27 16-28 17-35 18-29
20-22

ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 11-12 11-16 11-17 12-13
   12-20 13-14 14-15 15-16 17-18 18-19 19-20
exact/norm bonds :
1-32 2-31 3-30 6-37 7-21 11-17 12-20 13-24 14-25 15-27 16-28 17-18
17-35 18-19 18-29 19-20 20-22
exact bonds :
4-7 5-10 7-8 8-9 8-39 9-10 9-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
isolated ring systems :
containing 1 : 11 :

G1:C,H,O

G2:H,Cb,Cy,Hy

G3:C,H,O,Cb,Cy,Hy
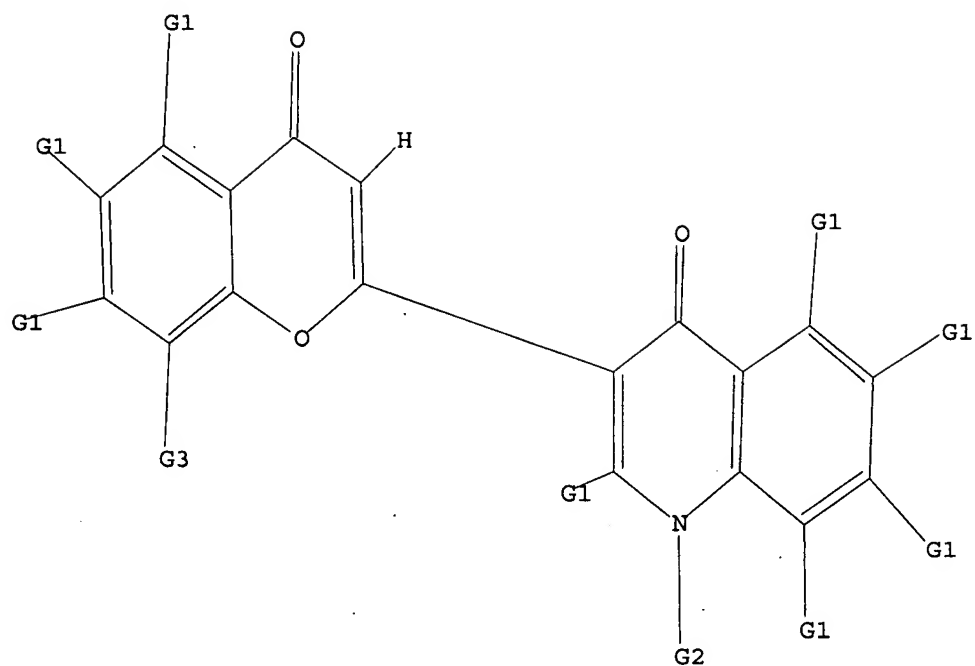
Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:CLASS 22:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 35:CLASS 37:CLASS 39:CLASS

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR

G1 C,H,O

G2 H,Cb,Cy,Hy

G3 C,H,O,Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 full

L3              21 SEA SSS FUL L1

=> file ca


=> s l3
L4               1 L3

=> d ibib abs fhitstr
```

L4   ANSWER 1 OF 1 CA COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 140:59525 CA
TITLE: Preparation of
3-(4-oxo-4H-chromen-2-yl)-(1H)-quinolin-
                           4-ones as anticancer agents
INVENTOR(S):   Brion, Jean Daniel; Israel, Lucien; Le Ridant, Alain;
                           Harpey, Catherine; Rabhi, Cherif; El Kaloun, Bachir
PATENT ASSIGNEE(S):   Les Laboratoires Servier, Fr.; Servier Lab
SOURCE: Fr. Demande, 36 pp.
                           CODEN: PRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2841243	A1	20031226	FR 2002-7536	20020619
FR 2841243	B1	20040820		
CA 2489136	A1	20031231	CA 2003-2489136	20030618
WO 2004000834	A1	20031231	WO 2003-FR1849	20030618

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
   CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
   GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
   LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
   PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
   UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
    KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
    FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
    BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003269003	A1	20040106	AU 2003-269003	20030618
EP 1513833	A1	20050316	EP 2003-750780	20030618
EP 1513833	B1	20060419		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
   IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

BR 2003011956	A	20050329	BR 2003-11956	20030618
CN 1692110	A	20051102	CN 2003-814050	20030618
JP 2005533077	T	20051104	JP 2004-514935	20030618
AT 323698	T	20060515	AT 2003-750780	20030618
PT 1513833	T	20060731	PT 2003-750780	20030618
ES 2263013	T3	20061201	ES 2003-1250780	20030618
NO 2004005540	A	20041217	NO 2004-5540	20041217
US 2006063801	A1	20060323	US 2004-519208	20041217

PRIORITY APPLN. INFO.:   FR 2002-7536   A 20020619

                                       WO 2003-FR1849   W 20030618

OTHER SOURCE(S):   MARPAT 140:59525
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L4   ANSWER 1 OF 1 CA COPYRIGHT 2007 ACS on STN   (Continued)
AB   Title compds. I [wherein R1, R2, R3, R4, R6, R8, R9, R10 = H, OH, alkyl,
     aryl/alkoxycarbonyl/alkoxy, arylalkoxy, and alkoxycarbonylalkoxy; R5 =
     alkyl, (un)substituted hetero/aryl; R7 = H, OH, alkoxy, cyclo/alkyl, or
R7
     = (un)substituted nitrogen or oxygen heterocycle; their optical isomers,
     pharmaceutical acceptable salts with acids, hydrates and solvates] were
     prepared as anticancer agents. For example, II was prepare by
esterification
     of 2,4-dimethoxy-6-hydroxyacetophenone (preparation given) with

2-acetyl-5-methoxyphenyl-4-oxo-1-phenyl-1,4-dihydroquinoline-3-carboxylate
     (preparation given), rearrangement in the presence of BuOK/DMF/THF,
cyclization
     in the presence of AcOH/H2SO4, and deprotection. In an in vitro
     cytotoxicity test, II showed an IC50 ranging from 0.25 µM to 0.05 µM
     towards five tumor cell lines. I exhibited a synergistic effect with
     several well-known anticancer agents (no data). Selected I induced
     apoptosis in 8 h.
IT   637362-92-6P, 3-(7-Methoxy-4-oxo-4H-1-benzopyran-2-yl)-1-phenyl-
     1,4-dihydroquinolin-4-one
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
     (anticancer agent; preparation of oxochromenylquinolinones as
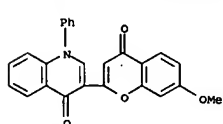anticancer
     agents)
RN   637362-92-6 CA
CN   4(1H)-Quinolinone, 3-(7-methoxy-4-oxo-4H-1-benzopyran-2-yl)-1-phenyl-
     (9CI) (CA INDEX NAME)

REFERENCE COUNT: 2   THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

```
=> file marpat
```

Expanded G-group definition display now available.

```
=> s l1 full
L5              1 SEA SSS FUL L1

=> d ibib abs fqhit
```

L5   ANSWER 1 OF 1   MARPAT   COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 140:59525 MARPAT
TITLE: Preparation of
3-(4-oxo-4H-chromen-2-yl)-(1H)-quinolin-
                           4-ones as anticancer agents
INVENTOR(S):   Brion, Jean Daniel; Israel, Lucien; Le Ridant, Alain;
                           Harpey, Catherine; Rabhi, Cherif; El Kaloun, Bachir
PATENT ASSIGNEE(S):   Les Laboratoires Servier, Fr.; Servier Lab
SOURCE: Fr. Demande, 36 pp.
                           CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2841243	A1	20031226	FR 2002-7536	20020619
FR 2841243	B1	20040820		
CA 2489136	A1	20031231	CA 2003-2489136	20030618
WO 2004000834	A1	20031231	WO 2003-FR1849	20030618

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
   CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
   GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
   LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
   PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
   UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
    KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
    FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
    BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003269003	A1	20040106	AU 2003-269003	20030618
EP 1513833	A1	20050316	EP 2003-750780	20030618
EP 1513833	B1	20060419		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
   IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

BR 200301956	A	20050329	BR 2003-11956	20030618
CN 1692110	A	20051102	CN 2003-814050	20030618
JP 2005533077	T	20051104	JP 2004-514935	20030618
AT 323698	T	20060515	AT 2003-750780	20030618
PT 1513833	T	20060731	PT 2003-750780	20030618
ES 2263013	T3	20061201	ES 2003-3750780	20030618
NO 2004005540	A	20041217	NO 2004-5540	20041217
US 2006063801	A1	20060323	US 2004-519208	20041217

PRIORITY APPLN. INFO.:   FR 2002-7536   20020619
                                          WO 2003-FR1849   20030618
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB   Title compds. I (wherein R1, R2, R3, R4, R6, R8, R9, R10 = H, OH, alkyl,
      aryl/alkoxycarbonyl/alkoxy, arylalkoxy, and alkoxycarbonylalkoxy; R5 =
      alkyl, (un)substituted hetero/aryl; R7 = H, OH, alkoxy, cyclo/alkyl, or
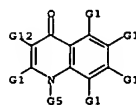R7

L5   ANSWER 1 OF 1   MARPAT   COPYRIGHT 2007 ACS on STN   (Continued)
      = (un)substituted nitrogen or oxygen heterocycle; their optical isomers,
      pharmaceutical acceptable salts with acids, hydrates and solvates) were
      prepd. as anticancer agents. For example, II was prep. by esterification
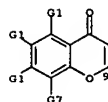   of 2,4-dimethoxy-6-hydroxyacetophenone (prepn. given) with

2-acetyl-5-methoxyphenyl-4-oxo-1-phenyl-1,4-dihydroquinoline-3-carboxylate
      (prepn. given), rearrangement in the presence of BuOK/DMF/THF,
cyclization
      in the presence of AcOH/H2SO4, and deprotection. In an in vitro
      cytotoxicity test, II showed an IC50 ranging from 0.25 µM to 0.05 µM
      towards five tumor cell lines. I exhibited a synergistic effect with
      several well-known anticancer agents (no data). Selected I induced
      apoptosis in 8 h.

MSTR 1

G1   = alkyl <containing 1-6 C>
G5   = carbocycle <containing 6-10 C, aromatic,
        6 or more normalized bonds, mono- or bicyclic,
        (1-2) 6-membered rings only> (opt. substd. by 1 or more G3)
G7   = alkyl <containing 1-6 C>
G12   = 9

Patent location: claim 1
Note: and pharmaceutically acceptable acid addition
                           salts, hydrates, and solvates
Note: also incorporates claim 10, formulas IV, V, VII,
                           and VIII
Note: additional ring formation also claimed
Stereochemistry: optical isomers

REFERENCE COUNT: 2   THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
                           RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

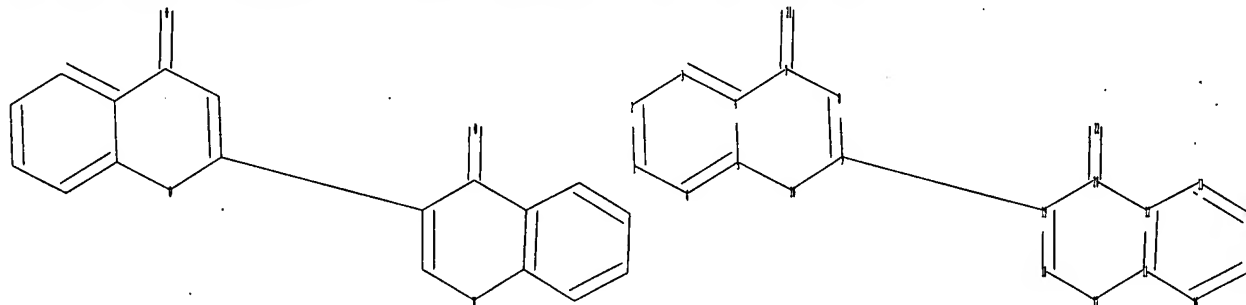L5   ANSWER 1 OF 1   MARPAT   COPYRIGHT 2007 ACS on STN   (Continued)

```
=> file reg

=>
Uploading C:\Program Files\Stnexp\Queries\11519208.str
```



```
chain nodes :
21  22
ring nodes :
1   2   3   4   5   6   7   8   9   10  11  12  13  14  15  16  17  18  19  20
chain bonds :
7-21   9-19   20-22
ring bonds :
1-2   1-6   2-3   3-4   4-5   4-7   5-6   5-10  7-8   8-9   9-10  11-12  11-16  11-17  12-13
 12-20  13-14  14-15  15-16  17-18  18-19  19-20
exact/norm bonds :
7-21   11-17   12-20   17-18   18-19   19-20   20-22
exact bonds :
4-7   5-10   7-8   8-9   9-10   9-19
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   11-12   11-16   12-13   13-14   14-15   15-16
isolated ring systems :
containing 1 : 11 :


G1:C,H,O

G2:H,Cb,Cy,Hy

G3:C,H,O,Cb,Cy,Hy

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom
20:Atom   21:CLASS   22:CLASS



L6        STRUCTURE  UPLOADED

=> d l6
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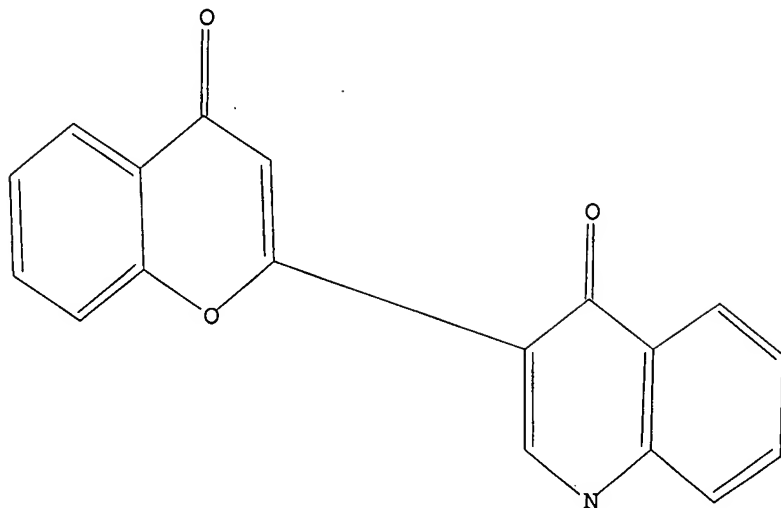
L6 HAS NO ANSWERS
L6   STR

G1 C,H,O

G2 H,Cb,Cy,Hy

G3 C,H,O,Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l6 full
L8   22 SEA SSS FUL L6

=> file ca

=> s l8
L9   1 L8

=> d his

     (FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007)

     FILE 'REGISTRY' ENTERED AT 11:07:14 ON 11 JUN 2007
L1   STRUCTURE UPLOADED
L2   1 S L1 SAM
L3   21 S L1 FULL

     FILE 'CA' ENTERED AT 11:07:41 ON 11 JUN 2007
 L4   1 S L3

     FILE 'MARPAT' ENTERED AT 11:07:49 ON 11 JUN 2007
L5   1 S L1 FULL

     FILE 'REGISTRY' ENTERED AT 11:08:05 ON 11 JUN 2007
L6   STRUCTURE UPLOADED

```
L7              1 S L6 SAM
L8              22 S L6 FULL

    FILE 'CA' ENTERED AT 11:09:02 ON 11 JUN 2007
L9              1 S L8

=> s l9 not l4
L10             0 L9 NOT L4

=> file reg

=>
Uploading C:\Program Files\Stnexp\Queries\12519208.str
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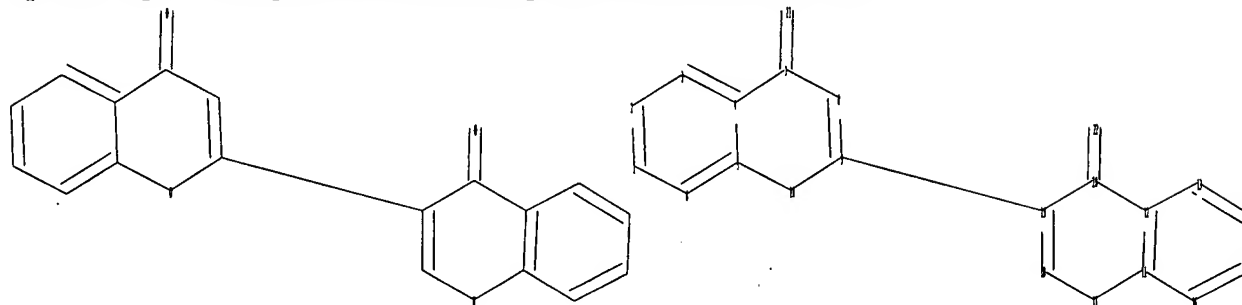


```
chain nodes :
21  22
ring nodes :
1   2   3   4   5   6   7   8   9   10  11  12  13  14  15  16  17  18  19  20
chain bonds :
7-21   9-19   20-22
ring bonds :
1-2   1-6   2-3   3-4   4-5   4-7   5-6   5-10   7-8   8-9   9-10   11-12   11-16   11-17   12-13
 12-20   13-14   14-15   15-16   17-18   18-19   19-20
exact/norm bonds :
4-7   5-10   7-8   7-21   8-9   9-10   11-17   12-20   17-18   18-19   19-20   20-22
exact bonds :
9-19
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   11-12   11-16   12-13   13-14   14-15   15-16


G1:C,H,O

G2:H,Cb,Cy,Hy

G3:C,H,O,Cb,Cy,Hy

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:CLASS  22:CLASS
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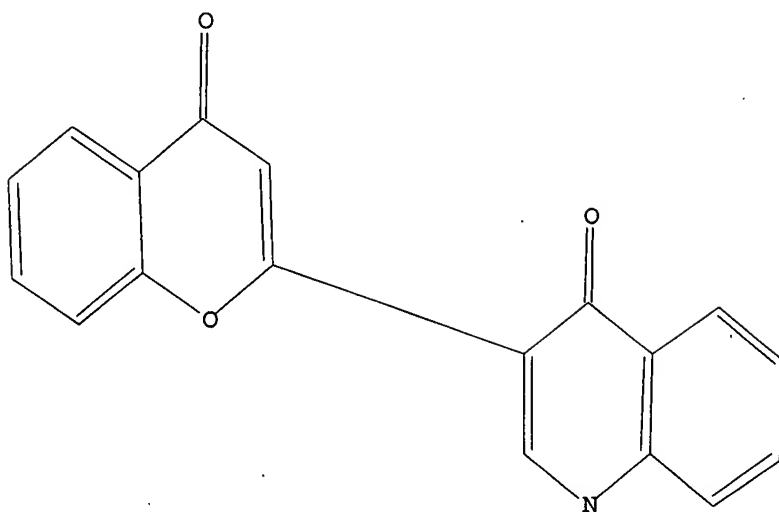
L11   STRUCTURE UPLOADED

=> d l11
L11 HAS NO ANSWERS
L11   STR

G1 C,H,O

G2 H,Cb,Cy,Hy

G3 C,H,O,Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l11 full
L12   22 SEA SSS FUL L11

=> d his

    (FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007)

    FILE 'REGISTRY' ENTERED AT 11:07:14 ON 11 JUN 2007
L1   STRUCTURE UPLOADED
L2   1 S L1 SAM
L3   21 S L1 FULL

    FILE 'CA' ENTERED AT 11:07:41 ON 11 JUN 2007
L4   1 S L3

    FILE 'MARPAT' ENTERED AT 11:07:49 ON 11 JUN 2007
L5   1 S L1 FULL

```
      FILE 'REGISTRY' ENTERED AT 11:08:05 ON 11 JUN 2007
L6                STRUCTURE UPLOADED
L7           1 S L6 SAM
L8          22 S L6 FULL


      FILE 'CA' ENTERED AT 11:09:02 ON 11 JUN 2007
L9           1 S L8
L10          0 S L9 NOT L4


      FILE 'REGISTRY' ENTERED AT 11:09:14 ON 11 JUN 2007
L11               STRUCTURE UPLOADED
L12         22 S L11 FULL

=> s l12 not l3
L13          1 L12 NOT L3

=> s l13 full
L14          1 L12 NOT L3

=> file ca

=> s l13
L15          1 L13

=> s l15 not l9
L16          0 L15 NOT L9

=> file marpat

=> d his

      (FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007)

      FILE 'REGISTRY' ENTERED AT 11:07:14 ON 11 JUN 2007
L1                STRUCTURE UPLOADED
L2           1 S L1 SAM
L3          21 S L1 FULL


      FILE 'CA' ENTERED AT 11:07:41 ON 11 JUN 2007
L4           1 S L3


      FILE 'MARPAT' ENTERED AT 11:07:49 ON 11 JUN 2007
L5           1 S L1 FULL


      FILE 'REGISTRY' ENTERED AT 11:08:05 ON 11 JUN 2007
L6                STRUCTURE UPLOADED
L7           1 S L6 SAM
L8          22 S L6 FULL


      FILE 'CA' ENTERED AT 11:09:02 ON 11 JUN 2007
L9           1 S L8
L10          0 S L9 NOT L4


      FILE 'REGISTRY' ENTERED AT 11:09:14 ON 11 JUN 2007
L11               STRUCTURE UPLOADED
L12         22 S L11 FULL
L13          1 S L12 NOT L3
```

```
L14              1 S L13 FULL

      FILE 'CA' ENTERED AT 11:10:24 ON 11 JUN 2007
L15              1 S L13
L16             . 0 S L15 NOT L9 ·

      FILE 'MARPAT' ENTERED AT 11:10:43 ON 11 JUN 2007

=> s l11 full
L17              1 SEA SSS FUL L11

=> file reg

=>
Uploading C:\Program Files\Stnexp\Queries\13519208.str
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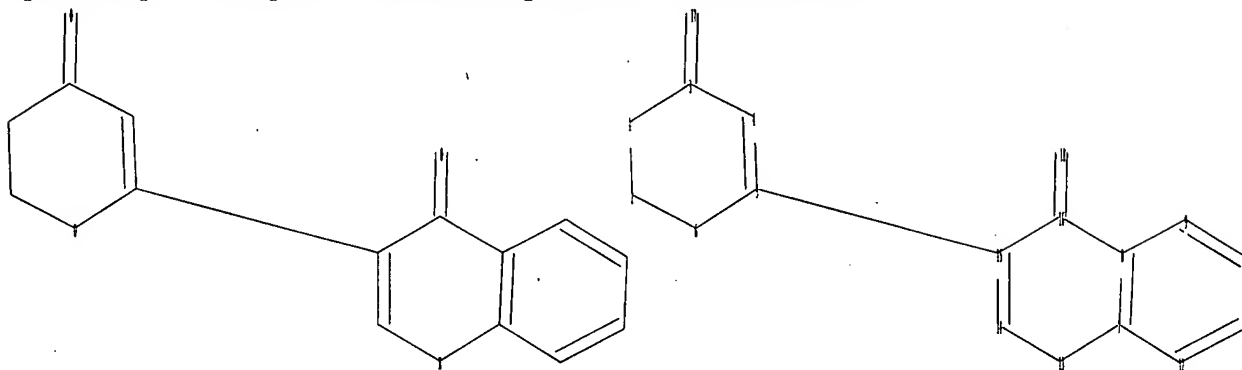


```
chain nodes :
17  18
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16
chain bonds :
3-17   5-15   16-18
ring bonds :
1-3  1-2  2-6  3-4  4-5  5-6  7-8  7-12  7-13  8-9  8-16  9-10  10-11  11-12  13-14
 14-15  15-16
exact/norm bonds :
1-3  1-2  2-6  3-4  3-17  4-5  5-6  7-13  8-16  13-14  14-15  15-16  16-18
exact bonds :
5-15
normalized bonds :
7-8  7-12  8-9  9-10  10-11  11-12


G1:C,H,O

G2:H,Cb,Cy,Hy

G3:C,H,O,Cb,Cy,Hy

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:CLASS  18:CLASS
```
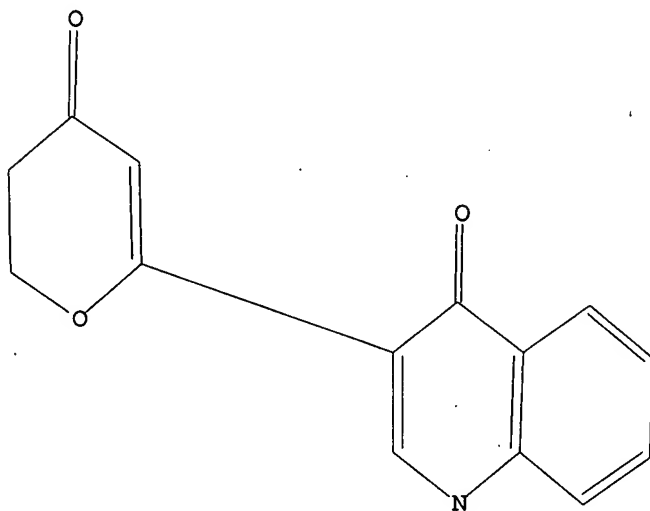
L18   STRUCTURE UPLOADED

```
=> d l18
L18 HAS NO ANSWERS
L18                 STR
```



```
G1 C,H,O
G2 H,Cb,Cy,Hy
G3 C,H,O,Cb,Cy,Hy
```

Structure attributes must be viewed using STN Express query preparation.

```
=> s l18 full
L19           22 SEA SSS FUL L18

=> d his

    (FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007)

    FILE 'REGISTRY' ENTERED AT 11:07:14 ON 11 JUN 2007
L1               STRUCTURE UPLOADED
L2          1 S L1 SAM
L3         21 S L1 FULL

    FILE 'CA' ENTERED AT 11:07:41 ON 11 JUN 2007
L4          1 S L3

    FILE 'MARPAT' ENTERED AT 11:07:49 ON 11 JUN 2007
L5          1 S L1 FULL

    FILE 'REGISTRY' ENTERED AT 11:08:05 ON 11 JUN 2007
```

```
L6                STRUCTURE UPLOADED
L7            1 S L6 SAM
L8           22 S L6 FULL

     FILE 'CA' ENTERED AT 11:09:02 ON 11 JUN 2007
L9            1 S L8
L10           0 S L9 NOT L4

     FILE 'REGISTRY' ENTERED AT 11:09:14 ON 11 JUN 2007
L11               STRUCTURE UPLOADED
L12          22 S L11 FULL
L13           1 S L12 NOT L3
L14           1 S L13 FULL

     FILE 'CA' ENTERED AT 11:10:24 ON 11 JUN 2007
L15           1 S L13
L16           0 S L15 NOT L9

     FILE 'MARPAT' ENTERED AT 11:10:43 ON 11 JUN 2007
L17           1 S L11 FULL

     FILE 'REGISTRY' ENTERED AT 11:11:07 ON 11 JUN 2007
L18               STRUCTURE UPLOADED
L19          22 S L18 FULL

=> s l19 not l12
L20           0 L19 NOT L12

=>

---Logging off of STN---


=>
Executing the logoff script...


=> LOG Y

STN INTERNATIONAL LOGOFF AT 11:12:25 ON 11 JUN 2007
```